

10/767,436

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NEWS 13 MAR 22 REGISTRY/ZREGISTRY enhanced with experimental property tags  
NEWS 14 APR 04 EPFULL enhanced with additional patent information and new  
fields  
NEWS 15 APR 04 EMBASE - Database reloaded and enhanced  
NEWS 16 APR 18 New CAS Information Use Policies available online  
  
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FILE 'HOME' ENTERED AT 18:14:29 ON 21 APR 2005

10/767,436

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STRUCTURE FILE UPDATES: 20 APR 2005 HIGHEST RN 848887-73-0

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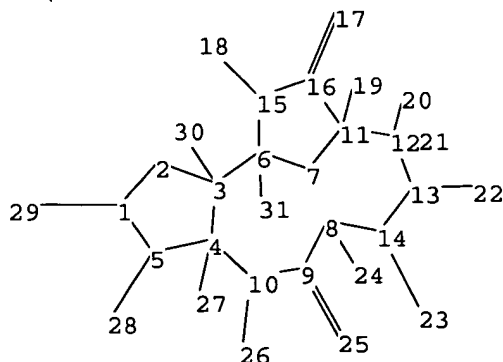
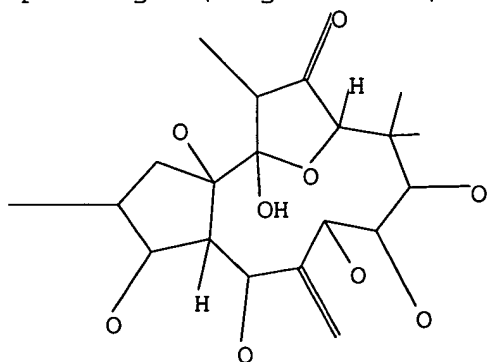
\*\*\*\*\*  
\*  
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=>

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chain nodes :

17 18 19 20 21 22 23 24 25 26 27 28 29 30 31

ring nodes :

1 2 3 4 5 6 7 8 9 10 11 12 13 14 15 16

10/767,436

chain bonds :

1-29 3-30 4-27 5-28 6-31 8-24 9-25 10-26 11-19 12-20 12-21 13-22 14-23  
15-18 16-17

ring bonds :

1-2 1-5 2-3 3-6 3-4 4-10 4-5 6-7 6-15 7-11 8-14 8-9 9-10 11-12 11-16  
12-13 13-14 15-16

exact/norm bonds :

3-30 5-28 6-31 8-24 10-26 13-22 14-23 16-17

exact bonds :

1-2 1-5 1-29 2-3 3-6 3-4 4-10 4-5 4-27 6-7 6-15 7-11 8-14 8-9 9-10  
9-25 11-12 11-16 11-19 12-13 12-20 12-21 13-14 15-16 15-18

isolated ring systems :

containing 1 :

Match level :

1:Atom 2:Atom 3:Atom 4:Atom 5:Atom 6:Atom 7:Atom 8:Atom 9:Atom 10:Atom  
11:Atom 12:Atom 13:Atom 14:Atom 15:Atom 16:Atom 17:CLASS 18:CLASS 19:CLASS  
20:CLASS 21:CLASS 22:CLASS 23:CLASS 24:CLASS 25:CLASS 26:CLASS 27:CLASS  
28:CLASS 29:CLASS 30:CLASS 31:CLASS

L1 STRUCTURE UPLOADED

=> s l1

SAMPLE SEARCH INITIATED 18:14:56 FILE 'REGISTRY'  
SAMPLE SCREEN SEARCH COMPLETED - 7 TO ITERATE

100.0% PROCESSED 7 ITERATIONS 0 ANSWERS  
SEARCH TIME: 00.00.01

FULL FILE PROJECTIONS: ONLINE \*\*COMPLETE\*\*  
BATCH \*\*COMPLETE\*\*  
PROJECTED ITERATIONS: 7 TO 298  
PROJECTED ANSWERS: 0 TO 0

L2 0 SEA SSS SAM L1

=> s l1 ful

FULL SEARCH INITIATED 18:15:02 FILE 'REGISTRY'  
FULL SCREEN SEARCH COMPLETED - 116 TO ITERATE

100.0% PROCESSED 116 ITERATIONS 7 ANSWERS  
SEARCH TIME: 00.00.01

L3 7 SEA SSS FUL L1

=> file caplus

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FILE COVERS 1907 - 21 Apr 2005 VOL 142 ISS 17  
FILE LAST UPDATED: 20 Apr 2005 (20050420/ED)

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=> s l3

L4 18 L3

=> d l4 ibib hitstr abs 1-18

L4 ANSWER 1 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:140078 CAPLUS

DOCUMENT NUMBER: 142:233304

TITLE: Diterpenes having cell division-inhibiting activity derived from Euphorbia kansui

INVENTOR(S): Kitanaka, Susumu; Miyata, Shohei; Wang, Li-Yan; Wang, Nai-Li; Yao, Sin-Sheng

PATENT ASSIGNEE(S): Nihon University, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 16 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2005041800	A2	20050217	JP 2003-201340	20030724
US 2005043549	A1	20050224	US 2004-767436	20040130
PRIORITY APPLN. INFO.:			JP 2003-201340	A 20030724

IT 57701-86-7P 672945-82-3P

RL: PAC (Pharmacological activity); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

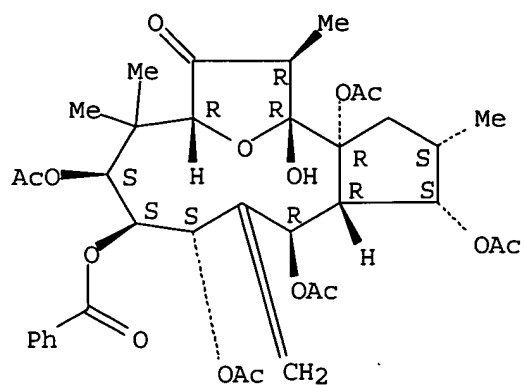
(isolation of diterpenes from Euphorbia kansui root and their cell division-inhibiting activity)

RN 57701-86-7 CAPLUS

CN 4,7-Epoxy-6H-cyclopentacyclododecene-6-one, 1,3a,9,11,13-pentakis(acetyloxy)-10-(benzoyloxy)tetradecahydro-4-hydroxy-2,5,8,8-tetramethyl-12-methylene-, (1S,2S,3aR,4R,5R,7R,9S,10S,11S,13R,13aR) - (9CI)  
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

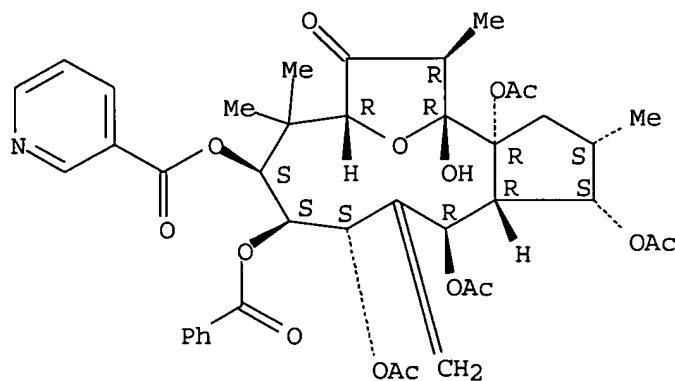
10/767,436



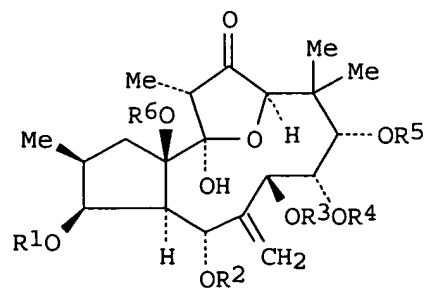
RN 672945-82-3 CAPLUS

CN 3-Pyridinecarboxylic acid, (1S,2S,3aR,4R,5R,7R,9S,10S,11S,13R,13aR) -  
1,3a,11,13-tetrakis (acetyloxy) -10- (benzoyloxy) tetradecahydro-4-hydroxy-  
2,5,8,8-tetramethyl-12-methylene-6-oxo-4,7-epoxy-1H-cyclopentacyclododecen-  
9-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



GI



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AB Diterpenes I [R1-R6 = H, (un)substituted (un)saturated linear or branched  
aliphatic group, COR; R = (un)substituted (un)saturated linear or branched  
aliphatic

group, (un)substituted aryl, (un)substituted heteroaryl], useful for treatment of malignant tumors such as esophageal cancer, breast cancer, etc., are claimed. Thus, 8 diterpenes were isolated from an EtOH extract of Euphorbia kansui root. Cell division-inhibiting activity of 2 of them were shown in Xenopus animal cap assay.

L4 ANSWER 2 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2005:140077 CAPLUS

DOCUMENT NUMBER: 142:212331

TITLE: Ingenol-type diterpene esters as cell division inhibitors

INVENTOR(S): Kitanaka, Susumu; Miyata, Shohei; Wang, Li-Yen; Wang, Nai-Li; Yao, Xin-Sheng

PATENT ASSIGNEE(S): Nihon University, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 16 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2005041799	A2	20050217	JP 2003-201339	20030724
PRIORITY APPLN. INFO.:			JP 2003-201339	20030724

IT 57701-86-7P 672945-82-3P

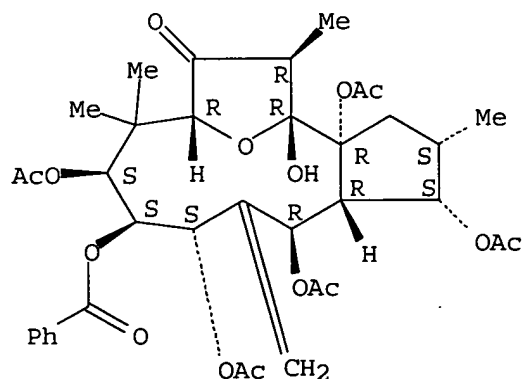
RL: PAC (Pharmacological activity); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(isolation of ingenol-type diterpene decadienoates from Euphorbia kansui root and their tumor cell division-inhibiting activity)

RN 57701-86-7 CAPLUS

CN 4,7-Epoxy-6H-cyclopentacyclododecene-6-one, 1,3a,9,11,13-pentakis(acetyloxy)-10-(benzoyloxy)tetradecahydro-4-hydroxy-2,5,8,8-tetramethyl-12-methylene-, (1S,2S,3aR,4R,5R,7R,9S,10S,11S,13R,13aR) - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

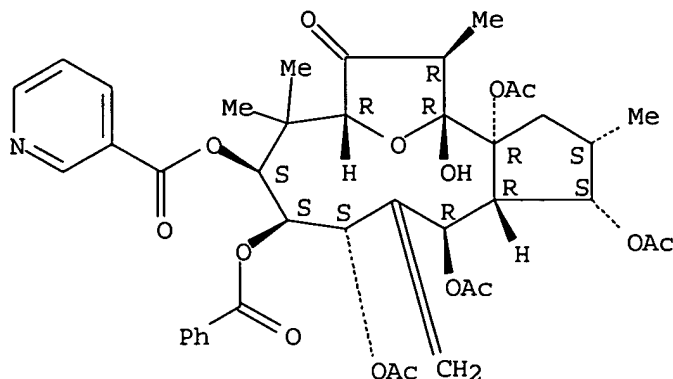


RN 672945-82-3 CAPLUS

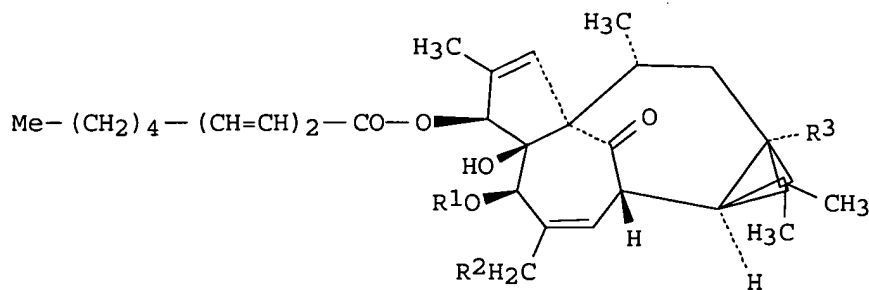
CN 3-Pyridinecarboxylic acid, (1S,2S,3aR,4R,5R,7R,9S,10S,11S,13R,13aR) - 1,3a,11,13-tetrakis(acetyloxy)-10-(benzoyloxy)tetradecahydro-4-hydroxy-2,5,8,8-tetramethyl-12-methylene-6-oxo-4,7-epoxy-1H-cyclopentacyclododecen-9-yl ester (9CI) (CA INDEX NAME)

10/767,436

Absolute stereochemistry.



GI



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AB The esters I [R1-R3 = H, (un)substituted (un)saturated linear or branched aliphatic group, COR; R = (un)substituted (un)saturated linear or branched aliphatic group, (un)substituted aryl, (un)substituted heteroaryl], useful for treatment of malignant tumors such as esophageal cancer, breast cancer, etc., are claimed. Thus, 8 diterpenes were isolated from an EtOH extract of *Euphorbia kansui* root. (E,E)-I (R1 = R2 = R3 = H) among them showed 55.1% cell division inhibition in *Xenopus* animal cap assay.

L4 ANSWER 3 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2004:668003 CAPLUS

DOCUMENT NUMBER: 141:328543

TITLE: Activity of Macrocyclic Jatrophone Diterpenes from *Euphorbia kansui* in a TrkA Fibroblast Survival Assay  
AUTHOR(S): Pan, Qin; Ip, Fanny C. F.; Ip, Nancy Y.; Zhu, Hua-Xu; Min, Zhi-Da

CORPORATE SOURCE: Department of Natural Medicinal Chemistry, China Pharmaceutical University, Nanjing, 210009, Peop. Rep. China

SOURCE: Journal of Natural Products (2004), 67(9), 1548-1551  
CODEN: JNPRDF; ISSN: 0163-3864

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

10/767,436

LANGUAGE: English

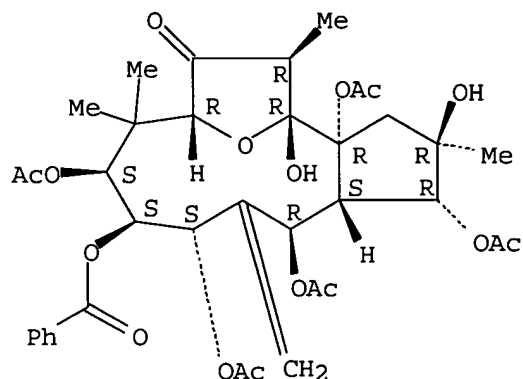
IT 770715-06-5P, Kansuinin H

RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)  
(macrocyclic jatrophone diterpenes from Euphorbia kansui)

RN 770715-06-5 CAPLUS

CN 4,7-Epoxy-6H-cyclopentacyclododecen-6-one, 1,3a,9,11,13-pentakis(acetyloxy)-10-(benzoyloxy)tetradecahydro-2,4-dihydroxy-2,5,8,8-tetramethyl-12-methylene-, (1R,2R,3aR,4R,5R,7R,9S,10S,11S,13R,13aS) - (9CI)  
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



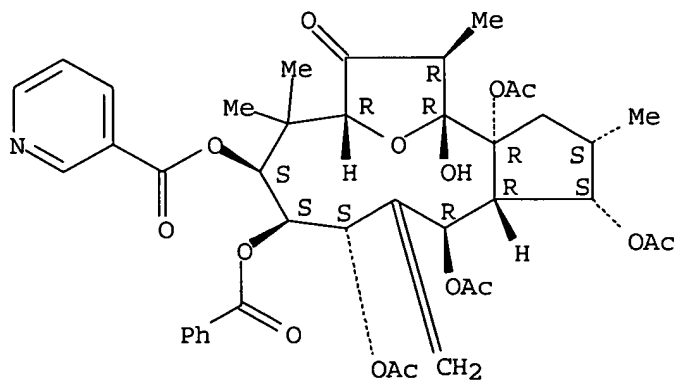
IT 672945-82-3P, Kansuinin D

RL: BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)  
(macrocyclic jatrophone diterpenes from Euphorbia kansui)

RN 672945-82-3 CAPLUS

CN 3-Pyridinecarboxylic acid, (1S,2S,3aR,4R,5R,7R,9S,10S,11S,13R,13aR) - 1,3a,11,13-tetrakis(acetyloxy)-10-(benzoyloxy)tetradecahydro-4-hydroxy-2,5,8,8-tetramethyl-12-methylene-6-oxo-4,7-epoxy-1H-cyclopentacyclododecen-9-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



IT 57701-86-7P, Kansuinin A

RL: BSU (Biological study, unclassified); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)



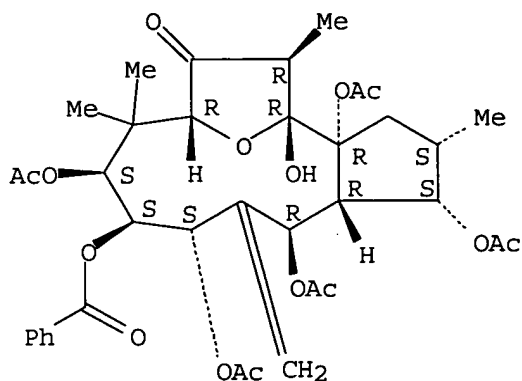
10/767,436

(macrocyclic jatrophone diterpenes from *Euphorbia kansui*)

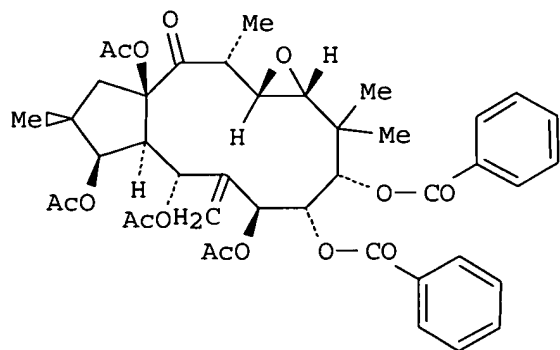
RN 57701-86-7 CAPLUS

CN 4,7-Epoxy-6H-cyclopentacyclododecene-6-one, 1,3a,9,11,13-pentakis(acetyloxy)-10-(benzoyloxy)tetradecahydro-4-hydroxy-2,5,8,8-tetramethyl-12-methylene-, (1S,2S,3aR,4R,5R,7R,9S,10S,11S,13R,13aR) - (9CI)  
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



GI



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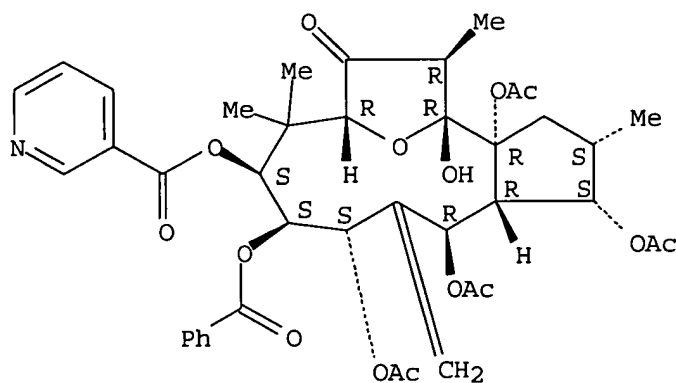
AB Three new macrocyclic diterpenes, kansuinins F (I), G, and H, together with four known jatrophone diterpenes, kansuinins D, E, and A and 3 $\beta$ ,5 $\alpha$ ,7 $\beta$ ,15 $\beta$ -tetraacetoxy-9 $\alpha$ -nicotinoyloxyjatropha-6(17)-11E-dien-14-one, were isolated from the roots of *Euphorbia kansui*. Kansuinins F and G were assigned as 6(17)-en-11,12-epoxy-14-one-type jatrophone diterpenes, and kansuinin H as a 6(17)-en-11,14-epoxy-12-one jatrophone diterpene. The structures of kansuinins F-H and the relative configurations of kansuinins D-E were determined by spectral data anal. Kansuinin E exhibited a specific survival effect on fibroblasts that expressed TrkA, a high-affinity receptor for nerve growth factor.

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 4 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:758409 CAPLUS  
 DOCUMENT NUMBER: 140:267543  
 TITLE: Studies on the bioactive constituents in euphorbiaceae. 3. Diterpenes from the roots of Euphorbia kansui and their in vitro effects on the cell division of Xenopus (2)  
 AUTHOR(S): Wang, Li-Yan; Wang, Nai-Li; Yao, Xin-Sheng; Miyata, Syohei; Kitanaka, Susumu  
 CORPORATE SOURCE: Department of Natural Products Chemistry, Shenyang Pharmaceutical University, Shenyang, 110016, Peop. Rep. China  
 SOURCE: Chemical & Pharmaceutical Bulletin (2003), 51(8), 935-941  
 CODEN: CPBTAL; ISSN: 0009-2363  
 PUBLISHER: Pharmaceutical Society of Japan  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 IT 672945-82-3P, Kansuinin D  
 RL: BSU (Biological study, unclassified); NPO (Natural product occurrence); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)  
 (diterpenes from the roots of Euphorbia kansui and their effect on the cell division)  
 RN 672945-82-3 CAPLUS  
 CN 3-Pyridinecarboxylic acid, (1S,2S,3aR,4R,5R,7R,9S,10S,11S,13R,13aR)-1,3a,11,13-tetrakis(acetyloxy)-10-(benzoyloxy)tetradecahydro-4-hydroxy-2,5,8,8-tetramethyl-12-methylene-6-oxo-4,7-epoxy-1H-cyclopentacyclododecen-9-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry.



AB Four new ingenane-type diterpenes, 3-O-(2,3-dimethylbutanoyl)-13-O-dodecanoyl-20-O-acetylingenol (1), 3-O-(2,3-dimethylbutanoyl)-13-O-dodecanoyl-20-deoxyingenol (2), 3-O-(2E,4Z-decadienoyl)-20-deoxyingenol (3), and 3-O-(2E,4E-decadienoyl)-20-deoxyingenol (4), two new jatrophane-type diterpenes, kansuins D (9) and E (10), and four known ingenane-type diterpenes were isolated from the root of Euphorbia kansui. Their structures were elucidated by spectroscopic and chemical anal., and individual Xenopus cells at the blastular stage were cultured with the diterpenes to test for biol. activity. 20-Deoxyingenol diterpenes 3 and 4 induced the greatest cell cleavage arrest (0.5 µg/mL of each compound resulted in >75% cleavage arrest), but cell cleavage inhibitory activity became weak when C-16 had an acyl residue. In contrast, the jatrophane diterpene kansuinin D showed no activity.

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REFERENCE COUNT: 17 THERE ARE 17 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 5 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:470467 CAPLUS

DOCUMENT NUMBER: 139:47129

TITLE: Diterpenes from Euphorbia kansui and compositions containing them as antiinflammatory or antitumor agents

INVENTOR(S): Kitanaka, Susumu; Miyata, Shohei

PATENT ASSIGNEE(S): Nihon University, Japan

SOURCE: Jpn. Kokai Tokkyo Koho, 13 pp.

CODEN: JKXXAF

DOCUMENT TYPE: Patent

LANGUAGE: Japanese

FAMILY ACC. NUM. COUNT: 1

PATENT INFORMATION:

PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 2003171349	A2	20030620	JP 2001-296613	20010927
PRIORITY APPLN. INFO.:			JP 2001-238341	A 20010806

IT 57701-86-7P

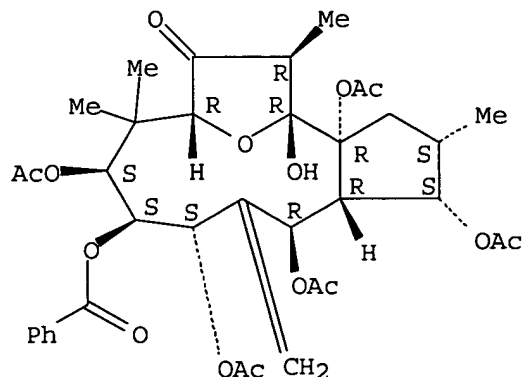
RL: PAC (Pharmacological activity); PUR (Purification or recovery); THU (Therapeutic use); BIOL (Biological study); PREP (Preparation); USES (Uses)

(isolation of diterpenes from Euphorbia kansui and their uses as anti-inflammatory or antitumor agents)

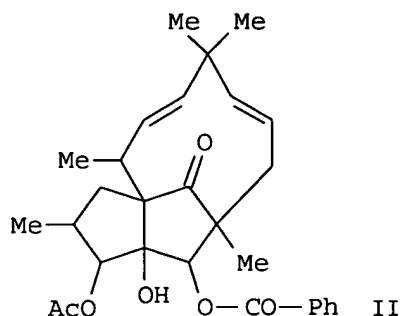
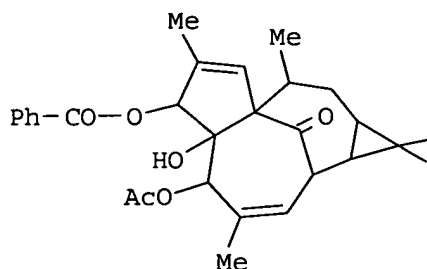
RN 57701-86-7 CAPLUS

CN 4,7-Epoxy-6H-cyclopentacyclododecene-6-one, 1,3a,9,11,13-pentakis(acetyloxy)-10-(benzoyloxy)tetradecahydro-4-hydroxy-2,5,8,8-tetramethyl-12-methylene-, (1S,2S,3aR,4R,5R,7R,9S,10S,11S,13R,13aR) - (9CI)  
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



GI



AB Compns. containing a diterpenes I are claimed. Also claimed are specific diterpenes II, III, IV, V, VI [R1 = H, R2 = (E,E)-CO(CH:CH)2(CH2)4Me], VI [R1 = H, R2 = (E,Z)-CO(CH:CH)2(CH2)4Me], VI [R1 = (E,E)-CO(CH:CH)2(CH2)4Me, R2 = H], VI [R1 = (E,Z)-CO(CH:CH)2(CH2)4Me, R2 = H], and VI [R1 = H, R2 = CO(CH2)8Me] and compns. containing them. The diterpenes are useful as antiinflammatory or antitumor agents. Root of *E. kansui* was extracted with EtOH and the EtOH extract was subsequently extracted with CHCl<sub>3</sub>, EtOAc, and BuOH 3 times for each solvent. The CHCl<sub>3</sub> fraction was concentrated and fractionated by silica gel column using gradient elution with hexane-EtOAc mixts. Isolation of above 10 diterpenes from the fractions were also shown. These diterpenes inhibited compound 48/80-induced histamine release from mast cells and inhibited cleavage of *Xenopus* late blastula.

L4 ANSWER 6 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2003:18338 CAPLUS

DOCUMENT NUMBER: 139:97906

TITLE: Studies on the structure of kansuine A from *Euphorbia kansui*

AUTHOR(S): Pan, Qin; Min, Zhi Da

CORPORATE SOURCE: Department of Natural Medicine Chemistry, China Pharmaceutical University, Nanjing, 210009, Peop. Rep. China

SOURCE: Chinese Chemical Letters (2002), 13(12), 1178-1180  
CODEN: CCLEE7; ISSN: 1001-8417

PUBLISHER: Chinese Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

IT 57701-86-7, Kansuine A

RL: PRP (Properties)

(Kansuinin A; structure of kansuine A from *Euphorbia kansui*)

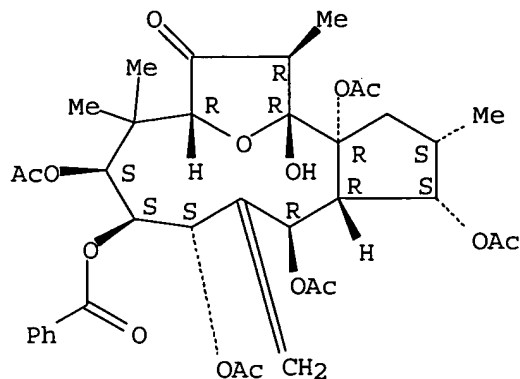
RN 57701-86-7 CAPLUS

CN 4,7-Epoxy-6H-cyclopentacyclododecene-6-one, 1,3a,9,11,13-

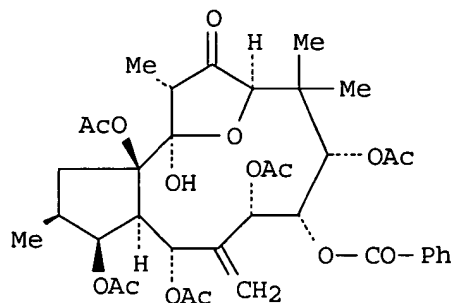
10/767,436

pentakis (acetyloxy) -10- (benzoyloxy) tetradecahydro-4-hydroxy-2,5,8,8-tetramethyl-12-methylene-, (1S,2S,3aR,4R,5R,7R,9S,10S,11S,13R,13aR) - (9CI)  
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



GI



I

AB Kansuine A (I) is a macrocyclic jatrophone diterpene that was isolated from *E. kansui*. Further investigation of the structure by HMQC, and HMBC spectra revealed that the benzoyl group is located at C-8 and an acetyl group is at C-3.

REFERENCE COUNT: 2 THERE ARE 2 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 7 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:569056 CAPLUS

DOCUMENT NUMBER: 137:275755

TITLE: Diterpenes from the roots of *Euphorbia kansui* and their in vitro effects on the cell division of *Xenopus*  
Wang, Li-Yan; Wang, Nai-Li; Yao, Xin-Sheng; Miyata, Syohei; Kitanaka, Susumu

CORPORATE SOURCE: Department of Natural Products Chemistry, Shenyang Pharmaceutical University, Shenyang, Shenhe District, 110016, Peop. Rep. China

SOURCE: Journal of Natural Products (2002), 65(9), 1246-1251  
CODEN: JNPRDF; ISSN: 0163-3864

10/767,436

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

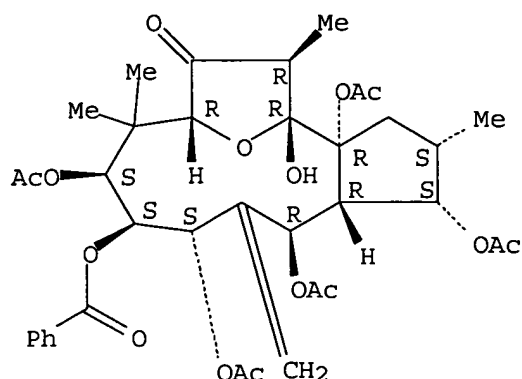
IT 57701-86-7, Kansuinin A

RL: BSU (Biological study, unclassified); BIOL (Biological study)  
(diterpenes from *Euphorbia kansui* and their in vitro effects on cell  
division of *Xenopus*)

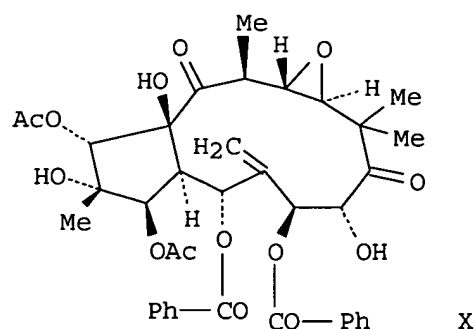
RN 57701-86-7 CAPLUS

CN 4,7-Epoxy-6H-cyclopentacyclododecene-6-one, 1,3a,9,11,13-  
pentakis(acetyloxy)-10-(benzoyloxy)tetradecahydro-4-hydroxy-2,5,8,8-  
tetramethyl-12-methylene-, (1S,2S,3aR,4R,5R,7R,9S,10S,11S,13R,13aR)- (9CI)  
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



GI



AB Twelve polycyclic diterpenes have been isolated from the roots of *Euphorbia kansui*. Nine were assigned with an ingenol skeleton, 20-O-(2'E,4'E-decadienoyl)ingenol (I), 20-O-(2'E,4'Z-decadienoyl)ingenol (II), 3-O-(2'E,4'Z-decadienoyl)ingenol (III), 3-O-(2'E,4'E-decadienoyl)ingenol (IV), 3-O-(2'E,4'Z-decadienoyl)-5-O-acetylingenol (V), 3-O-(2'E,4'Z-decadienoyl)-20-O-acetylingenol (VI), 3-O-(2'E,4'E-decadienoyl)-20-O-acetylingenol (VII), 20-O-(decanoyl)ingenol (VIII), and 5-O-(2'E,4'E-decadienoyl)ingenol (IX), and three with a jatropane skeleton, kansuinin A (XII), B (XI), and C (X). Compds. I, II, V, IX, and X are new compds., while IV and VII were assigned with new geometric

configurations. Their structures were elucidated by spectroscopic and chemical anal. In vitro treatment of cultured individual *Xenopus* cells at the blastular stage with I-IX arrested cleavage significantly (0.5 µg/mL of each compound resulted in >75% cleavage arrest). Of the three jatrophone diterpenes X-XII, only kansuinin B XI showed any activity, resulting in 87% cleavage arrest at 50 µg/mL.

REFERENCE COUNT: 25 THERE ARE 25 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 8 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 2002:284092 CAPLUS

DOCUMENT NUMBER: 137:179501

TITLE: New macrocyclic diterpenoids from *Euphorbia esula*

AUTHOR(S): Liu, L. G.; Meng, J. C.; Wu, S. X.; Li, X. Y.; Zhao, X. C.; Tan, R. X.

CORPORATE SOURCE: Institute of Functional Biomolecules, School of Life Sciences, Nanjing University, Nanjing, 210093, Peop. Rep. China

SOURCE: *Planta Medica* (2002), 68(3), 244-248

CODEN: PLMEAA; ISSN: 0032-0943

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

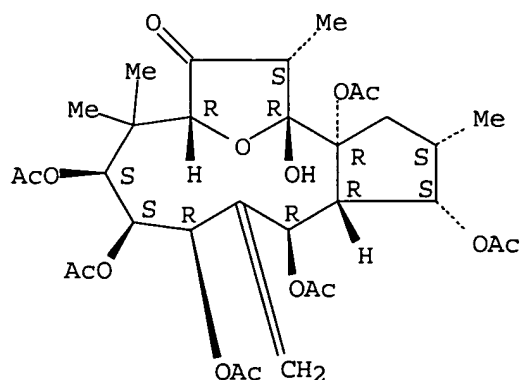
IT 449779-15-1P

RL: PAC (Pharmacological activity); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); PREP (Preparation)  
(new macrocyclic diterpenoids from *Euphorbia esula*)

RN 449779-15-1 CAPLUS

CN 4,7-Epoxy-6H-cyclopentacyclododecen-6-one, 1,3a,9,10,11,13-hexakis(acetyloxy)tetradecahydro-4-hydroxy-2,5,8,8-tetramethyl-12-methylene-, (1R,2R,3aS,4S,5R,7S,9R,10R,11S,13S,13aS)-rel-(+)-(9CI) (CA INDEX NAME)

Rotation (+). Absolute stereochemistry unknown.



AB The structures of two new macrocyclic jatrophone diterpenoid esters from the whole herb of *Euphorbia esula*, were established as 11,14-epoxy-3β,5α,7β,8α,9α,15β-hexaacetoxy-12-oxo-13αH-jatropha-6(17)-ene and 1α,3β-diacetoxy-5α,7β-dibenzoyloxy-9,14-dioxo-11β,12α-epoxy-2α,8α,15β-trihydroxy-13βH-jatropha-6(17)-ene by a combination of 1D- and 2D-NMR techniques as well as UV, IR and mass spectra data. Bioassay evaluation of all isolates against the human tumor cell lines (B16, KB, SMMC and BGC) indicated that the second ester was

cytotoxic to B16 with the IC50 value being 1.81 µg/mL. In addition, the irritant activity assay indicated that both diterpenoids were inactive (ID2450 > 100 µg/ear).

REFERENCE COUNT: 13 THERE ARE 13 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 9 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:43717 CAPLUS

DOCUMENT NUMBER: 130:129831

TITLE: Cytotoxicity and antiviral activity of the compounds from *Euphorbia kansui*

AUTHOR(S): Zheng, W. F.; Cui, Z.; Zhu, Q.

CORPORATE SOURCE: Laboratory Pharmacology Toxicology, Nanjing University Traditional Chinese Medicine, Nanjing, 210029, Peop. Rep. China

SOURCE: *Planta Medica* (1998), 64(8), 754-756

CODEN: PLMEAA; ISSN: 0032-0943

PUBLISHER: Georg Thieme Verlag

DOCUMENT TYPE: Journal

LANGUAGE: English

IT 57701-86-7, Kansuinin A

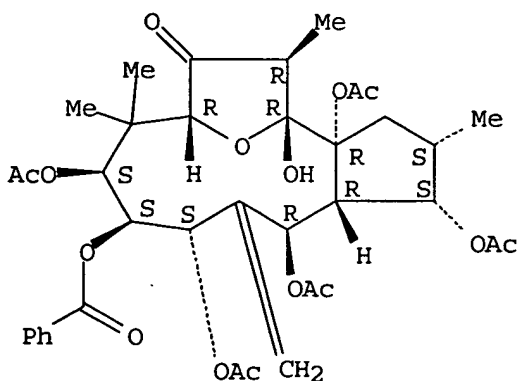
RL: BAC (Biological activity or effector, except adverse); BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); OCCU (Occurrence)

(cytotoxicity and antiviral activity of the compds. from *Euphorbia kansui*)

RN 57701-86-7 CAPLUS

CN 4,7-Epoxy-6H-cyclopentacyclododecene-6-one, 1,3a,9,11,13-pentakis(acetyloxy)-10-(benzoyloxy)tetradecahydro-4-hydroxy-2,5,8,8-tetramethyl-12-methylene-, (1S,2S,3aR,4R,5R,7R,9S,10S,11S,13R,13aR) - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



AB Eleven compds. including four triterpenes, one sterol, and six diterpenes from *E. kansui* had been assayed for their cytotoxicity and antiviral activity. The relations between structures and bioactivities have also been noted.

REFERENCE COUNT: 18 THERE ARE 18 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 10 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1999:15183 CAPLUS

DOCUMENT NUMBER: 130:213527



10/767,436

TITLE: Structure of esulol A, a novel macrocyclic diterpene, from inner Mongolian Euphorbia esula

AUTHOR(S): Sekine, Toshikazu; Kamiya, Minoru; Ikegami, Fumio; Qi, Jin-Feng

CORPORATE SOURCE: Faculty Pharmaceutical Sciences, Chiba University, Chiba, 263, Japan

SOURCE: Natural Product Letters (1998), 12(3), 237-239  
CODEN: NPLEEF; ISSN: 1057-5634

PUBLISHER: Harwood Academic Publishers

DOCUMENT TYPE: Journal

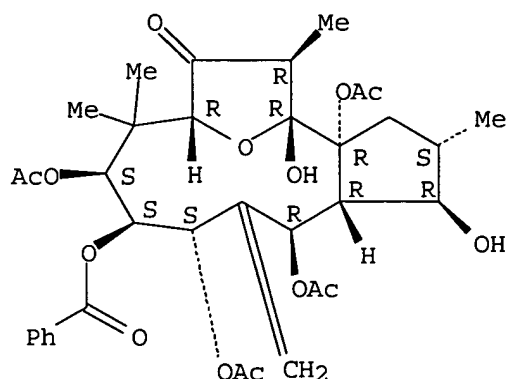
LANGUAGE: English

IT 221000-93-7, Esulol A  
RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); THU (Therapeutic use); BIOL (Biological study); OCCU (Occurrence); USES (Uses)  
(structure of esulol A, a novel macrocyclic diterpene, from inner Mongolian Euphorbia esula)

RN 221000-93-7 CAPLUS

CN 4,7-Epoxy-6H-cyclopentacyclododecen-6-one, 3a,9,11,13-tetrakis(acetyloxy)-10-(benzoyloxy)tetradecahydro-1,4-dihydroxy-2,5,8,8-tetramethyl-12-methylene-, (1R,2S,3aR,4R,5R,7R,9S,10S,11S,13R,13aR) - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



AB A new macrocyclic diterpene, esulol A was isolated from the aerial parts of Chinese Euphorbia esula (Euphorbiaceae). The relative structure was elucidated by spectroscopic analyses as a novel highly oxygenated jatrophane derivative

REFERENCE COUNT: 8 THERE ARE 8 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 11 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1998:573081 CAPLUS

DOCUMENT NUMBER: 129:273031

TITLE: Macrocyclic diterpene polyesters of the jatrophane type from Euphorbia esula

AUTHOR(S): Hohmann, Judit; Vasas, Andrea; Gunther, Gabor; Imre, Mathe; Ferenc, Evanics; Gyorgy, Dombi; Gyula, Jerkovich

CORPORATE SOURCE: Szoe Gyogynoveny, Drogismereti Intez., Szeged, 6701, Hung.

SOURCE: Acta Pharmaceutica Hungarica (1998), 68(3), 175-182  
CODEN: APHGAO; ISSN: 0001-6659

10/767,436

PUBLISHER: Magyar Gyogyszereszet Tarsasag

DOCUMENT TYPE: Journal

LANGUAGE: Hungarian

IT 188640-76-8P, Esulatin C

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study); OCCU (Occurrence); PREP (Preparation)

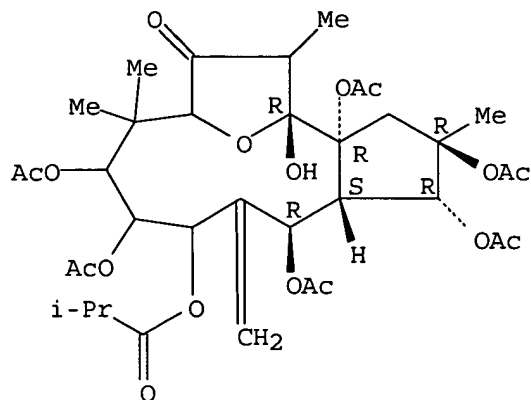
(macrocyclic diterpene polyesters of the jatrophone type from Euphorbia esula)

RN 188640-76-8 CAPLUS

CN Propanoic acid, 2-methyl-, (1R,2R,3aR,4R,13R,13aS)-1,2,3a,9,10,13-hexakis(acetyloxy)tetradecahydro-4-hydroxy-2,5,8,8-tetramethyl-12-methylene-6-oxo-4,7-epoxy-1H-cyclopentacyclododecen-11-yl ester (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

Currently available stereo shown.



AB Three new jatrophone diterpenes, esulatin A, B and C, were isolated and characterized from the whole, undried plant of Euphorbia esula. By means of spectral anal., the structures were established as penta- and heptaesters of previously unknown, polyfunctional diterpene parent alcs. Esculatin A and C are the diterpenoids with the highest degree of esterification identified to date from the family Euphorbiaceae.

L4 ANSWER 12 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1997:281032 CAPLUS

DOCUMENT NUMBER: 126:248838

TITLE: Macrocyclic Diterpene Polyesters of the Jatrophone Type from Euphorbia esula

AUTHOR(S): Hohmann, Judit; Vasas, Andrea; Guenther, Gabor; Mathe, Imre; Evanics, Ferenc; Dombi, Gyoergy; Jerkovich, Gyula

CORPORATE SOURCE: Department of Pharmacognosy, Albert Szent-Gyorgyi Medical University, Szeged, H-6701, Hung.

SOURCE: Journal of Natural Products (1997), 60(4), 331-335  
CODEN: JNPRDF; ISSN: 0163-3864

PUBLISHER: American Chemical Society

DOCUMENT TYPE: Journal

LANGUAGE: English

IT 188640-76-8P, Esulatin C

RL: BOC (Biological occurrence); BSU (Biological study, unclassified); PRP (Properties); PUR (Purification or recovery); BIOL (Biological study);

10/767,436

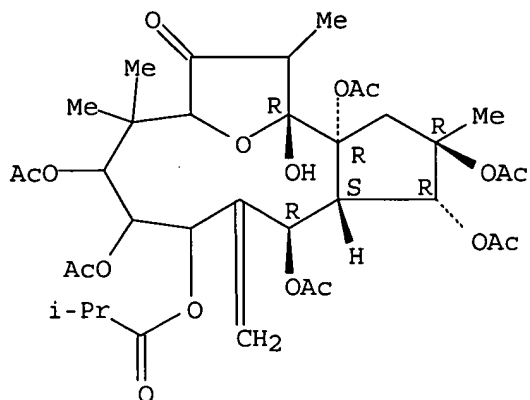
OCCU (Occurrence); PREP (Preparation)

(macrocyclic diterpene polyesters of the jatrophane type from *Euphorbia esula*)

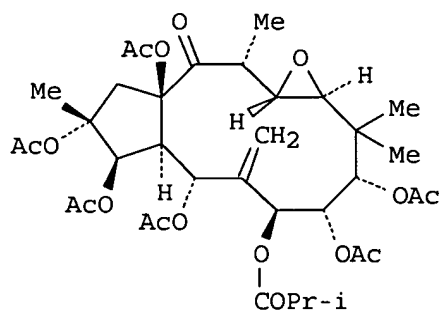
RN 188640-76-8 CAPLUS

CN Propanoic acid, 2-methyl-, (1R,2R,3aR,4R,13R,13aS)-1,2,3a,9,10,13-hexakis(acetyloxy)tetradecahydro-4-hydroxy-2,5,8,8-tetramethyl-12-methylene-6-oxo-4,7-epoxy-1H-cyclopentacyclododecen-11-yl ester (9CI) (CA INDEX NAME)

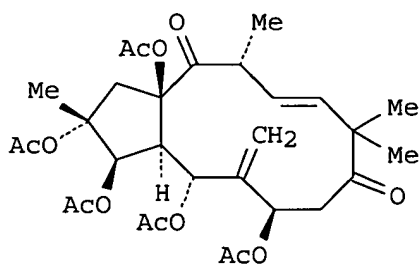
Absolute stereochemistry. Rotation (+).  
Currently available stereo shown.



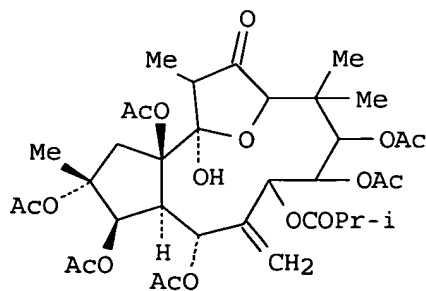
GI



I



II



III

AB Three new jatrophane diterpenes, esulatins A-C (I-III) were isolated and

characterized from the whole, undried plant of *Euphorbia esula*. By means of spectral anal., the structures were established as pentaesters and heptaesters of hitherto unknown, polyfunctional diterpene parent alcs. I and III are the diterpenoids with the highest degree of esterification identified to date from the family Euphorbiaceae.

REFERENCE COUNT: 15 THERE ARE 15 CITED REFERENCES AVAILABLE FOR THIS RECORD. ALL CITATIONS AVAILABLE IN THE RE FORMAT

L4 ANSWER 13 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1996:97985 CAPLUS

DOCUMENT NUMBER: 124:136518

TITLE: Cyclooxygenase induction is essential for NGF

synthesis enhancement by NGF inducers in L-M cells

AUTHOR(S): Yamaguchi, Kohji; Tsuji, Tomoko; Uemura, Daisuke; Kondo, Kiyosi

CORPORATE SOURCE: Sagami Chemical Research Center, Sagamihara, 229, Japan

SOURCE: Bioscience, Biotechnology, and Biochemistry (1996), 60(1), 92-4

CODEN: BBBIEJ; ISSN: 0916-8451

PUBLISHER: Japan Society for Bioscience, Biotechnology, and Agrochemistry

DOCUMENT TYPE: Journal

LANGUAGE: English

IT 57701-86-7, Kansuinin A

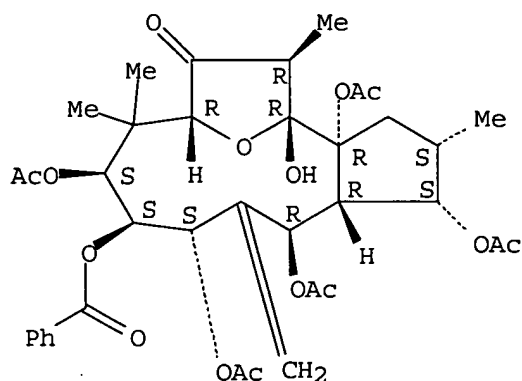
RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); BIOL (Biological study)

(cyclooxygenase induction requirement for NGF formation enhancement by NGF inducers in L-M cells)

RN 57701-86-7 CAPLUS

CN 4,7-Epoxy-6H-cyclopentacyclododecene-6-one, 1,3a,9,11,13-pentakis(acetyloxy)-10-(benzoyloxy)tetradecahydro-4-hydroxy-2,5,8,8-tetramethyl-12-methylene-, (1S,2S,3aR,4R,5R,7R,9S,10S,11S,13R,13aR) - (9CI) (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



AB Nerve growth factor (NGF) inducers, for example 4-methylcatechol, pyrroloquinoline quinone, kansuinin A, and ingenol triacetate, stimulate NGF synthesis in L-M cells, but the mechanism of NGF induction by NGF inducers is not known. Using the four different types of previously described NGF inducers, the authors proved induction of cyclooxygenase activity for NGF inducers and detected prostaglandins D2 and E2 as metabolites of arachidonic acid. From the observation that the induction

of NGF by each NGF inducers was inhibited by cyclooxygenase inhibitors or dexamethasone, cyclooxygenase activation is apparently an essential process for NGF induction.

L4 ANSWER 14 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1995:759318 CAPLUS  
 DOCUMENT NUMBER: 123:218433  
 TITLE: Nerve growth factor formation promoters containing diterpenes from Euphorbia  
 INVENTOR(S): Tsuji, Tomoko; Yamaguchi, Koji; Kamimura, Daisuke; Kondo, Sei  
 PATENT ASSIGNEE(S): Sagami Chem Res, Japan  
 SOURCE: Jpn. Kokai Tokkyo Koho, 5 pp.  
 CODEN: JKXXAF  
 DOCUMENT TYPE: Patent  
 LANGUAGE: Japanese  
 FAMILY ACC. NUM. COUNT: 1  
 PATENT INFORMATION:

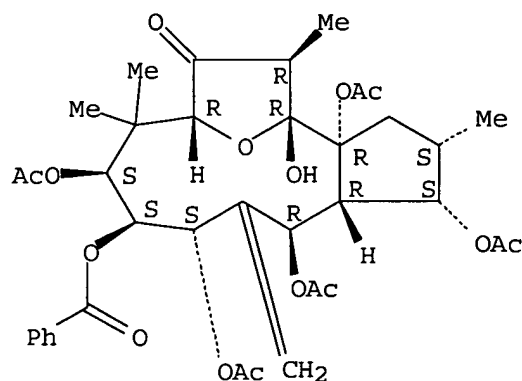
PATENT NO.	KIND	DATE	APPLICATION NO.	DATE
JP 07149633	A2	19950613	JP 1993-319187	19931126

PRIORITY APPLN. INFO.: JP 1993-319187 19931126

IT **57701-86-7**, Kansuinin A  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (NGF formation promoters containing kansuinin A, triacetylingenol, or jolkinolide B for treatment of nerve disorders)

RN 57701-86-7 CAPLUS  
 CN 4,7-Epoxy-6H-cyclopentacyclododecene-6-one, 1,3a,9,11,13-pentakis(acetyloxy)-10-(benzoyloxy)tetradecahydro-4-hydroxy-2,5,8,8-tetramethyl-12-methylene-, (1S,2S,3aR,4R,5R,7R,9S,10S,11S,13R,13aR) - (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).

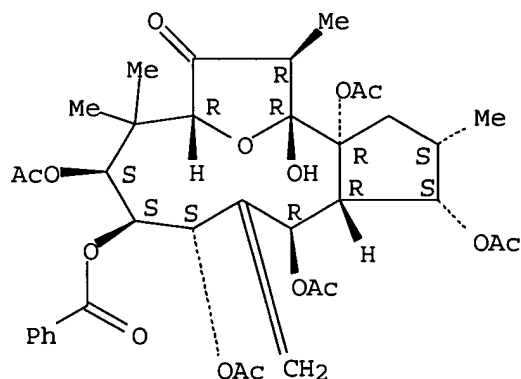


AB NGF formation promoters containing kansuinin A (I), triacetylingenol, and/or jolkinolide B as active ingredients are claimed. The promoters are useful for treatment of spinal injury, peripheral nerve injury, diabetic neuropathy, and amyotrophic lateral sclerosis. NGF formation by ML cell was increased 120 times by addition of I at 50 µg/mL.

L4 ANSWER 15 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1994:646113 CAPLUS  
 DOCUMENT NUMBER: 121:246113  
 TITLE: Stimulation of nerve growth factor production by diterpenoids isolated from plants of Euphorbia species  
 AUTHOR(S): Yamaguchi, Kohji; Uemura, Daisuke; Tsuji, Tomoko; Kondo, Kiyosi  
 CORPORATE SOURCE: Sagami Chem. Res. Center, Kanagawa, 229, Japan  
 SOURCE: Bioscience, Biotechnology, and Biochemistry (1994), 58(9), 1749-51  
 CODEN: BBBIEJ; ISSN: 0916-8451  
 DOCUMENT TYPE: Journal  
 LANGUAGE: English  
 IT 57701-86-7, Kansuinin A  
 RL: BAC (Biological activity or effector, except adverse); BSU (Biological study, unclassified); THU (Therapeutic use); BIOL (Biological study); USES (Uses)  
 (stimulation of nerve growth factor production by diterpenoids isolated from plants of Euphorbia species)  
 RN 57701-86-7 CAPLUS  
 CN 4,7-Epoxy-6H-cyclopentacyclododecene-6-one, 1,3a,9,11,13-pentakis(acetyloxy)-10-(benzoyloxy)tetradecahydro-4-hydroxy-2,5,8,8-tetramethyl-12-methylene-, (1S,2S,3aR,4R,5R,7R,9S,10S,11S,13R,13aR)- (9CI)  
 (CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



AB Kansuinin A, ingenol triacetate, and jolkinolide B, diterpenoids isolated from Euphorbia, were potent inducers of nerve growth factor production in L-M cells. Each of these compds. has unique characteristics in the potency of the activity and the range of ED. Kansuinin A had the strongest activity, ingenol triacetate had wide-range activity, and jolkinolide B had narrow-range activity.

L4 ANSWER 16 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN  
 ACCESSION NUMBER: 1975:593546 CAPLUS  
 DOCUMENT NUMBER: 83:193546  
 TITLE: Toxic substances of Euphorbiaceae  
 AUTHOR(S): Hirata, Yoshimasa  
 CORPORATE SOURCE: Dep. Chem., Nagoya Univ., Nagoya, Japan  
 SOURCE: Pure and Applied Chemistry (1975), 41(1-2), 175-99  
 CODEN: PACHAS; ISSN: 0033-4545  
 DOCUMENT TYPE: Journal; General Review  
 LANGUAGE: English  
 IT 57701-86-7P

10/767,436

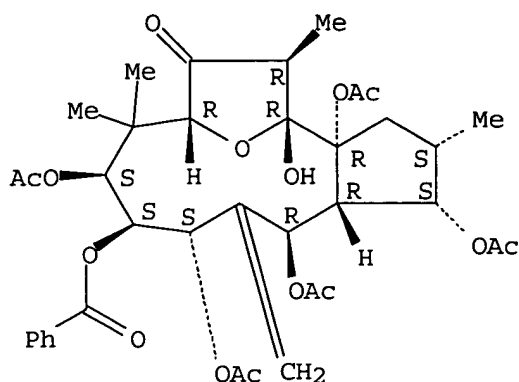
RL: PREP (Preparation)

(from Euphorbia kansui, mol. structure of)

RN 57701-86-7 CAPLUS

CN 4,7-Epoxy-6H-cyclopentacyclododecene-6-one, 1,3a,9,11,13-pentakis(acetyloxy)-10-(benzoyloxy)tetradecahydro-4-hydroxy-2,5,8,8-tetramethyl-12-methylene-, (1S,2S,3aR,4R,5R,7R,9S,10S,11S,13R,13aR) - (9CI)  
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



GI For diagram(s), see printed CA Issue.

AB Kansuine A (3,5,8,9-tri-O-acetyl-mono-O-benzoyl-I) and B (II) were isolated from Euphorbia kansui. The structure of I was determined from chemical

and spectral data and that of II from chemical and spectral data and by x-ray anal. of the p-bromobenzoate III formed from II by successive treatment with OsO<sub>4</sub> and p-BrC<sub>6</sub>H<sub>4</sub>COCl. Crystals of III were of space group P1 with a 10.57, b 11.97, c 9.96 Å, α 103.3, β 104.1, and γ 82.2°. The structure, biosynthesis, and biol. properties of the alkaloids and terpenoids from the family Euphorbiaceae were reviewed.

L4 ANSWER 17 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1975:497621 CAPLUS

DOCUMENT NUMBER: 83:97621

TITLE: Structure of kansuine A, a new multi-oxygenated diterpene

AUTHOR(S): Uemura, Daisuke; Hirata, Yoshimasa; Chen, Yuh-Pan; Hsu, Hong-Yen

CORPORATE SOURCE: Chem. Inst., Nagoya Univ., Nagoya, Japan

SOURCE: Tetrahedron Letters (1975), (21), 1697-700

CODEN: TELEAY; ISSN: 0040-4039

DOCUMENT TYPE: Journal

LANGUAGE: English

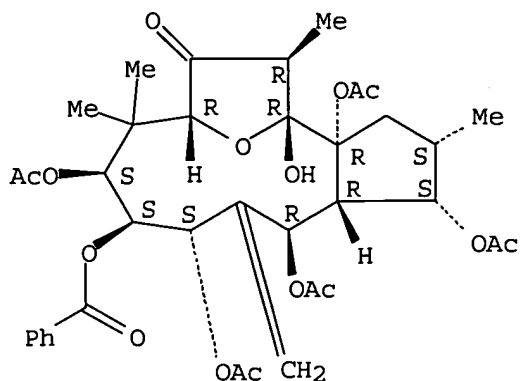
IT 57701-86-7

RL: RCT (Reactant); RACT (Reactant or reagent)  
(of Euphorbia kansui, structure of)

RN 57701-86-7 CAPLUS

CN 4,7-Epoxy-6H-cyclopentacyclododecene-6-one, 1,3a,9,11,13-pentakis(acetyloxy)-10-(benzoyloxy)tetradecahydro-4-hydroxy-2,5,8,8-tetramethyl-12-methylene-, (1S,2S,3aR,4R,5R,7R,9S,10S,11S,13R,13aR) - (9CI)  
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



GI For diagram(s), see printed CA Issue.

AB The structure of kansuine A, a tri-O-acetyl-O-benzoyl derivative (14-OH unacylated) of the pentaol I, extracted from *Euphorbia kansui*, was determined from chemical and spectral data.

L4 ANSWER 18 OF 18 CAPLUS COPYRIGHT 2005 ACS on STN

ACCESSION NUMBER: 1975:479401 CAPLUS

DOCUMENT NUMBER: 83:79401

TITLE: Stereochemistry of kansuine A

AUTHOR(S): Uemura, Daisuke; Hirata, Yoshimasa

CORPORATE SOURCE: Chem. Inst., Nagoya Univ., Nagoya, Japan

SOURCE: Tetrahedron Letters (1975), (21), 1701-2

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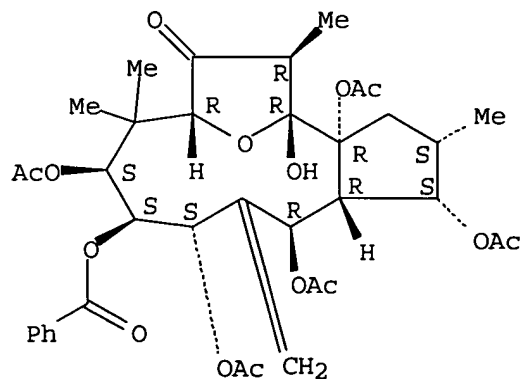
IT 57701-86-7

RL: RCT (Reactant); RACT (Reactant or reagent)  
(stereochem. of)

RN 57701-86-7 CAPLUS

CN 4,7-Epoxy-6H-cyclopentacyclododecene-6-one, 1,3a,9,11,13-pentakis(acetyloxy)-10-(benzoyloxy)tetradecahydro-4-hydroxy-2,5,8,8-tetramethyl-12-methylene-, (1S,2S,3aR,4R,5R,7R,9S,10S,11S,13R,13aR) - (9CI)  
(CA INDEX NAME)

Absolute stereochemistry. Rotation (+).



GI For diagram(s), see printed CA Issue.

AB The stereochem. of kansuine A, a tri-O-acetyl-O-benzoyl derivative (14-OH



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unacylated) of the pentaol I, was determined from chemical and spectral data.

=> log y

COST IN U.S. DOLLARS

SINCE FILE

TOTAL

ENTRY

SESSION

FULL ESTIMATED COST

89.37

250.91

DISCOUNT AMOUNTS (FOR QUALIFYING ACCOUNTS)

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TOTAL

ENTRY

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